

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.25 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.00e-01

Confidence level: 4.89e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Methyl-2,4-pentanediol</div> <div>Measured: 2.86</div> <div>Predicted: 1.35e-02</div>	<div>Image not found</div> <div>1-Methylpyrrole</div> <div>Measured: 4.00e-01</div> <div>Predicted: 11.0</div>	<div>Image not found</div> <div>3-Methylpentane</div> <div>Measured: 4.50e-01</div> <div>Predicted: 124</div>
<div>Image not found</div> <div>Nitralin</div> <div>Measured: 7.61</div> <div>Predicted: 1.77e-08</div>		